Weakly-Interacting Bosons in a Trap within Approximate Second Quantization Approach

Andrij Rovenchak

Department for Theoretical Physics, Ivan Franko National University of Lviv, 12 Drahomanov St., Lviv, UA–79005, Ukraine

The theory of Bogoliubov is generalized for the case of a weakly-interacting Bose-gas in harmonic trap. A set of nonlinear matrix equations is obtained to make the diagonalization of Hamiltonian possible. Its perturbative solution is used for the calculation of the energy and the condensate fraction of the model system to show the applicability of the method.

PACS numbers: 03.75.Hh, 05.30.−d

1. INTRODUCTION

In recent decades, the experimental achievements in the investigation of ultra-cold alkali gases[1,2] revived the interest to theoretical models of bosonic systems[3]. The quantum field-theoretical techniques occupy a predominant position within the methods for the studies of weakly-interacting bosons. The creation–annihilation operator formalism was directly applied in Refs. 4,5,6. The use of nonlinear Schrödinger equation (Gross–Pitaevskii equation) is much more popular for the studies in this domain[7]. Some modifications[8] and extensions[9] of this methods are also available. Numerical techniques were utilized by Krauth[10], Pearson et al.[11] and may others. The low-dimensional Bose-systems became of special interest recently[11,12,13,14].

In this work, a method similar to that of Bogoliubov[4] is developed for a weakly-interacting D-dimensional Bose-gas in the harmonic trapping potential. The paper is organized as follows. In the next Section, the Hamiltonian of the system under study is written in the approximate second quantization approach. As a result of its diagonalization a set of matrix equations is obtained. The results of calculations of the condensate fraction and energy are given in Section 3.

2. HAMILTONIAN DIAGONALIZATION

We consider a D-dimensional system of N weakly-interacting bosons of mass m confined in the harmonic trap

$$V(x_1,\ldots,x_D)=\frac{m}{2}\left(\omega_1^2x_1^2+\ldots+\omega_D^2x_D^2\right). \tag{1}$$

The potential of interatomic interaction is given by $U(x_1,\ldots,x_D)=g\delta(\mathbf{x})$, where the vector $\mathbf{x}=(x_1,\ldots,x_D)$, g is the interaction strength.

The Hamiltonian reads

$$\hat{H}=\sum_{j=1}^{N}\left[\frac{\hat{\mathbf{p}}_j^2}{2m}+V(\mathbf{x}_j)\right]+\sum_{1\le j<l\le N}U(\mathbf{x}_j-\mathbf{x}_l)=\hat{H}_0+\hat{U}. \tag{2}$$

Here, $\hat{\mathbf{p}}_j$ is the momentum operator of the jth particle, $\mathbf{x}_j$ is its coordinate.

It is possible to develop the second quantization approach using the eigenfunctions $|\mathbf{n}\rangle=|n_1,\ldots,n_D\rangle$ of the operator $\hat{H}_0$, i. e., an ordinary D-dimensional harmonic oscillator. For simplicity, we further demand that no ratio of the frequencies $\omega_1,\ldots,\omega_D$ is a rational number to avoid an accidental degeneration of energy levels.

Let $\hat{a}^\dagger_{\mathbf{n}},\hat{a}_{\mathbf{n}}$ be the creation and annihilation operators for the state $|\mathbf{n}\rangle$. The corresponding energy levels are $\varepsilon_{\mathbf{n}}=\hbar\left(\omega_1n_1+\ldots+\omega_Dn_D\right)$. In this representation the Hamiltonian (2) is

$$\hat{H}=\sum_{\mathbf{n}}\varepsilon_n\hat{a}^\dagger_{\mathbf{n}}\hat{a}_{\mathbf{n}}+\frac{1}{2}\sum_{\mathbf{m},\mathbf{m}',\mathbf{n},\mathbf{n}'}\langle\mathbf{mn}|U|\mathbf{m}'\mathbf{n}'\rangle\hat{a}^\dagger_{\mathbf{m}}\hat{a}^\dagger_{\mathbf{n}}\hat{a}_{\mathbf{m}'}\hat{a}_{\mathbf{n}'}. \tag{3}$$

The operators satisfy standard bosonic commutation relations:

$$\left[\hat{a}_{\mathbf{n}'},\hat{a}^\dagger_{\mathbf{n}}\right]=\delta_{\mathbf{nn}'} \tag{4}$$

Now we apply an approximate second quantization procedure following Bogoliubov[4]. Let N_0 be the number of particles at the lowest energy level ε_0. As the interaction is weak, the behaviour of bosons does not differ much from that of an ideal system. That is, one can expect the Bose–Einstein condensation to occur at low temperatures. The number N_0 is thus a macroscopic number. As it is an eigenvalue of the operator $\hat{a}^\dagger_0\hat{a}_0$, one can treat $\hat{a}^\dagger_0$ and $\hat{a}_0$ as c-numbers: $\hat{a}^\dagger_0\hat{a}_0=N_0$, $\hat{a}_0\hat{a}^\dagger_0=N_0+1\simeq N_0$, $\hat{a}^\dagger_0\simeq\sqrt{N_0}$, $\hat{a}_0\simeq\sqrt{N_0}$. To obtain more general results we do not put here $N_0=N$. Note, that for $D<3$ the condensation appears only in traps[15].

Further, following Bogoliubov, we neglect the terms having more than two operators with non-zero index. As the eigenfunctions $|\mathbf{n}\rangle$ are real the

matrix elements in the second item of (3) at different operator combinations are equal: $\langle \mathbf{m0}|U|\mathbf{n0}\rangle = \langle \mathbf{mn}|U|\mathbf{00}\rangle = \langle \mathbf{00}|U|\mathbf{mn}\rangle \equiv g\, c_{\mathbf{mn}}$, where

$$c_{\mathbf{mn}} = \left(\frac{m\omega}{2\pi^2\hbar}\right)^{D/2} \prod_{j=1}^{D} (-1)^{(3m_j+n_j)/2} \frac{1}{\sqrt{m_j!\, n_j!}}\, \Gamma\left(\frac{m_j+n_j+1}{2}\right) \tag{5}$$

if $m_j + n_j$ is even for all j and $c_{\mathbf{mn}} = 0$ otherwise. The notation $\omega = (\omega_1 \ldots \omega_D)^{\frac{1}{D}}$.

The matrix elements with three zeros equal

$$\langle \mathbf{n0}|U|\mathbf{00}\rangle \equiv g\, d_{\mathbf{n}} = g\left(\frac{m\omega}{2\pi^2\hbar}\right)^{D/2} \prod_{j=1}^{D} (-1)^{n_j/2} \frac{1}{\sqrt{n_j!}}\, \Gamma\left(\frac{n_j+1}{2}\right) \tag{6}$$

if n_j is even for all j.

The Hamiltonian (3) becomes

$$\begin{aligned} \hat{H} &= \text{const} + \sum_{\mathbf{n}} \varepsilon_{\mathbf{n}} \hat{a}^\dagger_{\mathbf{n}} \hat{a}_{\mathbf{n}} + g N_0^{3/2} \sum_{\mathbf{n}} d_{\mathbf{n}} \left(\hat{a}^\dagger_{\mathbf{n}} + \hat{a}_{\mathbf{n}}\right) \\ &\quad + g\, \frac{N_0}{2} \sum_{\mathbf{m},\mathbf{n}} c_{\mathbf{mn}} \left(4\hat{a}^\dagger_{\mathbf{m}} \hat{a}_{\mathbf{n}} + \hat{a}^\dagger_{\mathbf{m}} \hat{a}^\dagger_{\mathbf{n}} + \hat{a}_{\mathbf{m}} \hat{a}_{\mathbf{n}}\right), \end{aligned} \tag{7}$$

where 'const' denotes the items of a non-operator nature. Hereafter, it will be dropped. For brevity, the conditions $\mathbf{n} \neq 0, \mathbf{m} \neq 0$ is not written explicitly. Note the appearance of linear terms $\sim \hat{a}^\dagger, \sim \hat{a}$ which were absent in Bogoliubov's approach[4] due to the momentum conservation law.

Let the indices m, n run over all the states denoted by vector indices $\mathbf{m}, \mathbf{n}$. In order to obtain an energy spectrum of the Hamiltonian from Eq. (7) we will try to diagonalize it. For this purpose, it is possible to write (7) in the following matrix form:

$$\hat{H} = \hat{\mathbf{a}}^\dagger \mathcal{E} \hat{\mathbf{a}} + 2\lambda\sqrt{N_0}\left(\hat{\mathbf{a}}^\dagger \mathbf{d} + \hat{\mathbf{a}}^T \mathbf{d}\right) + \lambda\left(4\hat{\mathbf{a}}^\dagger C \hat{\mathbf{a}} + \hat{\mathbf{a}}^\dagger C \hat{\mathbf{a}}^{\dagger T} + \hat{\mathbf{a}}^T C \hat{\mathbf{a}}\right) \tag{8}$$

In the above equation, $\hat{\mathbf{a}}$ and $\mathbf{d}$ are vectors of infinite dimension:

$$\hat{\mathbf{a}}^T = (\hat{a}_1,\, \hat{a}_2\, \ldots), \qquad \hat{\mathbf{a}}^\dagger = \left(\hat{a}^\dagger_1,\, \hat{a}^\dagger_2,\, \ldots\right), \quad \mathbf{d}^T = (d_1,\, d_2,\, \ldots),$$

The diagonal matrix $\mathcal{E} = \begin{pmatrix} \varepsilon_1 & 0 & 0 & \ldots \\ 0 & \varepsilon_2 & 0 & \cdots \\ \vdots & & \ddots & \end{pmatrix}$, and the matrix elements of C are the coefficients c_{mn}. We have also written $g\, N_0/2 = \lambda$ for brevity.

In order to obtain the Hamiltonian in a diagonal form,

$$\hat{H} = \sum_n \epsilon_n \hat{\alpha}^\dagger_n \hat{\alpha}_n = \hat{\boldsymbol{\alpha}}^\dagger \mathfrak{E}\, \hat{\boldsymbol{\alpha}}, \tag{9}$$

where $\mathfrak{E}$ is the diagonal matrix with elements ϵ_n, one can apply a generalization of the well-known Bogoliubov's u–v transformation demanding

$$\hat{\mathbf{a}} = X\hat{\boldsymbol{\alpha}} + Y\hat{\boldsymbol{\alpha}}^{\dagger T} + \mathbf{z}, \qquad \hat{\mathbf{a}}^{\dagger} = \hat{\boldsymbol{\alpha}}^{\dagger}X + \hat{\boldsymbol{\alpha}}^{T}Y + \mathbf{z}^{T}. \tag{10}$$

Here, X and Y are square matrices of infinite dimension, we will require them to be Hermitian (symmetric and real), and $\mathbf{z}$ is a vector with real components. From the commutation relation (4) one can show that matrices X and Y obey the following condition

$$X^2 - Y^2 = I, \tag{11}$$

where I is a unit matrix.

It is easy to show that the linear terms (the expressions in the first parenthesis) of (8) produce only a shift of the energy levels but do not affect the distance between them. That is why hereafter we consider only the quadratic in $\hat{\mathbf{a}}$ and $\hat{\boldsymbol{\alpha}}$ terms of the Hamiltonian.

To eliminate the linear in $\hat{\boldsymbol{\alpha}}$ terms from $\hat{H}$, the vector $\mathbf{z}$ must be

$$\mathbf{z} = -2\lambda\sqrt{N_0}\,(\mathcal{E} + 6\lambda C)^{-1}\mathbf{d}. \tag{12}$$

Demanding the terms $\hat{\alpha}_m^{\dagger}\hat{\alpha}_n^{\dagger}$ and $\hat{\alpha}_m\hat{\alpha}_n$ to vanish in the Hamiltonian one gets the following matrix equations:

$$X\mathcal{E}Y + 4\lambda XCY + \lambda XCX + \lambda YCY = 0, \tag{13}$$

$$Y\mathcal{E}X + 4\lambda YCX + \lambda XCX + \lambda YCY = 0. \tag{14}$$

The matrix $\mathfrak{E}$ is

$$\mathfrak{E} = X\mathcal{E}X + Y\mathcal{E}Y + 4\lambda(XCX + YCY) + 2\lambda(XCY + YCX) \tag{15}$$

and its eigenvalues define the energy spectrum.

If the interatomic interaction is turned off ($g = 0$), the solutions are $X = I,\ Y = 0$. We will expand the matrices X and Y into series over λ:

$$X = I + 2\lambda^2\chi^2 + \ldots, \qquad Y = \lambda\upsilon + \lambda^2\upsilon_1 + \ldots\ . \tag{16}$$

The matrices $\chi, \upsilon, \upsilon_1$ can be found from Eqs. (11)–(14):

$$\upsilon = 2\chi; \qquad \chi = -\mathcal{E}^{-1}C/2; \qquad \upsilon_1 = 4\,\mathcal{E}^{-1}C\mathcal{E}^{-1}C. \tag{17}$$

In the approximation up to λ^2 we obtain the matrix $\mathfrak{E}$:

$$\mathfrak{E} = \mathcal{E} + 4\lambda C + \frac{\lambda^2}{2}\left\{\left(\mathcal{E}^{-1}C\right)^2\mathcal{E} - 3\,C\mathcal{E}^{-1}C - 2\mathcal{E}^{-1}C^2\right\} \tag{18}$$

and the energy levels are given by $\epsilon_n = \varepsilon_n + 4\lambda c_{nn} + \mathcal{O}(\lambda^2)$.

Equations (11)–(14) are difficult to solve, being non-linear with respect to infinite matrices. This set may be treated as coupled algebraic (matrix) Riccati equations:

$$XAY + XBX + YBY = 0, \tag{19}$$

$$YAX + XBX + YBY = 0, \tag{20}$$

$$X^2 - Y^2 - I = 0, \tag{21}$$

where $A = \mathcal{E} + 4\lambda C,\ B = \lambda C$. The numerical (non-perturbative) solution of this set needs special approaches[16]. This problem will be considered in a separate paper.

3. CALCULATION RESULTS

If Bose–Einstein condensation occurs, the chemical potential μ of the system approaches zero and the total number of particles is given by

$$N = N_0 + \sum_{n>0} \frac{1}{\exp(\epsilon_n/T) - 1}, \tag{22}$$

where N_0 is the occupation of the lowest energy level. Therefore, given N and the energy spectrum $\epsilon_n = \epsilon_n(\lambda) = \epsilon_n(gN_0)$ from the eigenvalues of (18), one can calculate N_0 as a function of temperature T. We thus arrive at a self-consistent problem. Its solution allows one to calculate the energy

$$E = E_0 + \sum_{n>0} \frac{\epsilon_n}{\exp(\epsilon_n/T) - 1} \tag{23}$$

and other thermodynamic functions.

In Fig. 1 the dependencies of the condensate fraction N_0/N and energy $(E - E_0)/N$ on temperature are given for the 1D gas. For simplicity, the following values of parameters are used in the calculations: $\hbar = \omega = 1,\ m = 2\pi^2,\ N = 1000,\ g = 0.0002$.

Since $c_{nn} > 0$, the interaction shifts the energy levels up, which effectively corresponds to lighter particles. Thus, the Bose-condensation temperature increases. Note, however, that the presented approach is not valid for higher temperatures as more items must be included in the Hamiltonian (7).

To summarize, the Bogoliubov's idea of an approximate second quantization approach is generalized for a weakly-interacting Bose-gas confined in a harmonic trap. As a result, the equations permitting to diagonalize the Hamiltonian and to calculate the elementary excitation spectrum are obtained. A perturbative solution is applied and the condensate fraction and energy dependencies on temperature are calculated for a model system to demonstrate the validity of the approach.

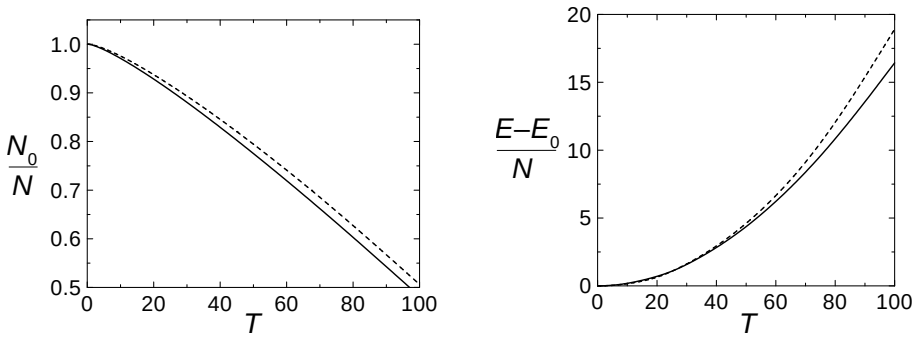

Fig. 1. (left) — Condensate fraction N_0/N as a function of temperature T; (right) — energy as a function of temperature. Dashed line is the interacting system, solid line is the ideal Bose-gas.

Acknowledgements. I am grateful to my colleagues from the Dept. for Theoretical Physics, Natl. University of Lviv, for valuable comments and discussions, in particular to Prof. Ivan Vakarchuk, Prof. Volodymyr Tkachuk, Taras Fityo, Yuri Krynytskyi. I wish also to express my gratitude to Prof. Beatrice Meini, University of Pisa, and to Dr. Hiroaki Mukaidani, Hiroshima University, for their helpful comments on the matrix equations treatment.

REFERENCES

1. M. H. Anderson et al., *Science* **269**, 198 (1995).
2. K. B. Davis et al., *Phys. Rev. Lett.* **75**, 3969 (1995).
3. C. J. Pethick and H. Smith, *Bose–Einstein Condensation in Dilute Gases* (Cambridge, Cambridge University Press), (2001).
4. N. N. Bogoliubov, *J. Phys. USSR* **11**, 23 (1947).
5. W. H. Bassichis and L. L. Foldy, *Phys. Rev.* **133**, A935 (1964).
6. M. Okumura and Y. Yamanaka, *Phys. Rev. A* **68**, 013609 (2003).
7. F. Dalfovo et al., *Rev. Mod. Phys.* **71**, 463 (1999); J. O. Andersen, *Rev. Mod. Phys.* **76**, 599 (2004); R. Ozeri et al., *Rev. Mod. Phys.* **77**, 187 (2005).
8. H. Fu, Y. Wang and B. Gao, *Phys. Rev. A* **67**, 053612 (2003).
9. E. B. Kolomeisky et al., *Phys. Rev. Lett.* **85**, 1146 (2000).
10. W. Krauth, *Phys. Rev. Lett.* **77**, 3695 (1996).
11. S. Pearson, T. Pang and C. Chen, *Phys. Rev. A* **58**, 1485 (1998).
12. N. J. van Druten and W. Ketterle, *Phys. Rev. Lett.* **79**, 549 (1997).
13. K. V. Kheruntsyan et al., *Phys. Rev. A* **71**, 053615 (2005).
14. M. T. Batchelor et al., *J. Phys. A* **38** 7787 (2005).
15. V. Bagnato and D. Kleppner, *Phys. Rev. A* **44**, 7439 (1991).
16. N. Bessis and G. Bessis, *J. Math. Phys.* **38** 5483 (1997); B. Meini, *Lin. Alg. Appl.* **413** 440 (2006); H. Mukaidani and T. Shimomura, *J. Math. Analysis Appl.* **267**, 209 (2002).